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Uncertainty for Part Density Determination: An Update

By

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Abstract

Accurate and precise density measurements by hydrostatic weighing requires the use of an analytical balance, configured with a suspension system, to both measure the weight of a part in water and in air. Additionally, the densities of these liquid media (water and air) must be precisely known for the part density determination. To validate the accuracy and precision of these measurements, uncertainty statements are required. The work in this report is a revision of an original report written more than a decade ago, specifically applying principles and guidelines suggested by the *Guide to the Expression of Uncertainty in Measurement (GUM)* for determining the part density uncertainty through sensitivity analysis. In this work, updated derivations are provided; an original example is revised with the updated derivations and appendix, provided solely to uncertainty evaluations using Monte Carlo techniques, specifically using the NIST Uncertainty Machine, as a viable alternative method.

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1.0 Introduction

The following report is an updated approach to the estimation of the measurement uncertainty associated with part density determination first developed by Martinez [1] more than a decade ago. A systematic approach will adhere to the guidelines recommended by the *Guide to the Expression of Uncertainty in Measurement* (GUM) [2] where a measurement model will be utilized and a sensitivity analysis performed. Probability distributions for each uncertainty contribution will be determined using reasonable justifications from statistical analysis and/or published literature.

2.0 Background

Classical part density is determined using the relationship between the part's *true mass* and *true volume*. Regrettably, it is not possible to exactly know these values, as there are random and systematic errors which contribute to the uncertainty of a particular quantity. As an alternative, *conventional true values* can be utilized but determining these conventional values with very low uncertainty is an arduous task, requires high-precision measurements taken with high-precision instrumentation. Therefore, the modern and most accurate method is measurements performed via hydrostatic weighing for density determination where measurement (mathematical) models can be determined [3], thus providing the most reliable method.

The theory goes as follows: a part's *conventional weight*, $\overline{W}$, is measured in media with different densities, where the conventional weight is defined as the difference between the weight from the gravitational load exerted by one medium (air) and the weight from the buoyant force exerted by the other medium (water). Thus one gets conventional weights of the part in medium one (air) and medium two (water) as determined by Eq. 1,

$$\begin{aligned} \overline{W}_A &= g(M - \rho_A V) \qquad (in\ air) \\ \overline{W}_W &= g(M - \rho_W V) \qquad (in\ water) \end{aligned} \tag{1}$$

Determination of the conventional values for $\overline{W}_A$ and $\overline{W}_W$ is done via the averaging of a series of measurements. From these average measurements, values for ρ_A (density of air) and ρ_W (density of water) can be calculated, solving Eq. 1 simultaneously as a system of equations. As a result, the measurement model of the part's density is shown in Eq. 2 below,

$$\rho_O = f(W_A, W_W, \rho_W, \rho_A) = \frac{W_A \rho_W - W_W \rho_A}{W_A - W_W} \tag{2}$$

For clarity, mass and weight are considered synonymous in this work; therefore, weight will be the preferred term. Also, the parameter nomenclature of $\bar{W}$ is treated synonymously with W, hence W is the term of choice, as seen in Eq. 2.

3.0 Uncertainty

Measurement uncertainty is defined in the VIM as *"non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurand, based on the information used"* [4]. To estimate measurement uncertainty, the GUM suggests a systematic process of stating the measurand, realizing the measurand, modeling the measurand with all known influence quantities, calculating the sensitivity coefficients of each influence quantity, determining standard uncertainties for each influence quantity, calculating the combined standard uncertainty and calculating the expanded uncertainty for a known confidence interval. An additional suggestion is that all known systematic biases be corrected beforehand, thus limiting influences to randomness and unknown systematic contributors. Although very procedural, the GUM is very dense in information but alternative resources that reflect the GUM principles are available [5] which take a more focused approach. The objective of this report is the sensitivity analysis and evaluation of the combined standard uncertainty.

3.1 Part Density Uncertainty

With the measurement model defined in Eq. 2, the combined standard uncertainty can be modeled using *The Law of Propagation of Uncertainty* (LPU) from the GUM, which is modeled below in Eq. 3,

$$u_c(f) = \left[\sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + \underbrace{2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left(\frac{\partial f}{\partial x_i}\right)\left(\frac{\partial f}{\partial x_j}\right)u(x_i, x_j)}_{correlation\ term}\right]^{1/2} \tag{3}$$

where the second term is the correlation term if two or more quantities are interdependent. This should not be ignored if known influence quantities correlate or if there is no ideal way to eliminate interdependency.

Since the measurement model is a function of weights and densities, both of whose values are determined using *different* techniques (i.e., weights via a mass balance system and densities through the use of derived formulae), it is acceptable to assume that there is no correlation between influence quantities. Therefore, the *correlation term* in Eq. 2 is equal to zero. Hence, the uncertainty model for the parts density is determined using Eq. 4,

$$u_c(\rho_O) = \left[\left(\frac{\partial\rho_O}{\partial W_A}\right)^2 u^2(W_A) + \left(\frac{\partial\rho_O}{\partial\rho_W}\right)^2 u^2(\rho_W) + \left(\frac{\partial\rho_O}{\partial W_W}\right)^2 u^2(W_W) + \left(\frac{\partial\rho_O}{\partial\rho_A}\right)^2 u^2(\rho_A)\right]^{1/2} \quad (4).$$

Calculation of the sensitivity coefficients is shown below in Eq. 5,

$$\begin{gathered}
\frac{\partial\rho_O}{\partial W_A} = \frac{W_W(\rho_A - \rho_W)}{(W_A - W_W)^2} \\
\frac{\partial\rho_O}{\partial\rho_W} = \frac{W_A}{W_A - W_W} \\
\frac{\partial\rho_O}{\partial W_W} = \frac{W_A(\rho_W - \rho_A)}{(W_A - W_W)^2} \\
\frac{\partial\rho_O}{\partial\rho_A} = -\frac{W_W}{W_A - W_W}
\end{gathered} \quad (5).$$

The sensitivity coefficients measure how sensitive the measurand is to each influence quantity. To do this, partial derivatives are utilized as a means to evaluate *individual* variation. The opposite is true for total derivatives where all quantities are allowed to vary *simultaneously*, leading to a larger uncertainty value as some of the terms may be accounted for more than once. After computation of the sensitivity coefficients, substitution into Eq. 4 yields the model for the combined standard uncertainty of the part density, Eq. 6,

$$\begin{aligned}
u_c(\rho_O) = \Bigg[&\left(\frac{W_W(\rho_A - \rho_W)}{(W_A - W_W)^2}\right)^2 u^2(W_A) + \left(\frac{W_A}{W_A - W_W}\right)^2 u^2(\rho_W) + \cdots \\
&+ \left(\frac{W_A(\rho_W - \rho_A)}{(W_A - W_W)^2}\right)^2 u^2(W_W) + \left(-\frac{W_W}{W_A - W_W}\right)^2 u^2(\rho_A)\Bigg]^{1/2}
\end{aligned} \quad (6).$$

The use of a measurement model shows the relationship of indirect measurements, which converts potentially multiple, individual values into the corresponding value of the measurand of interest, therefore the ability to estimate a near-complete solution of the measurement uncertainty. However, this method does not take into account the uncertainty contribution from the measurement process itself. Errors from the measurement process can be the result of intrinsic and extrinsic factors which affect the measurement result systematically and randomly. Accounting for these measurement process errors into an uncertainty contribution is done through experimental data, specifically repeated measurements [6]. With that in mind, the *total uncertainty* is estimated by adding in quadrature the combined standard uncertainty, determined by sensitivity analysis, and the sample standard deviation of the repeated measurements (measurement process), $s(MP)$ as shown in Eq. 7 below,

$$u_{Total}(\rho_O) = [u_c^2(\rho_O) + s^2(MP)]^{1/2} \tag{7}$$

3.2 Standard Uncertainties

To complete the uncertainty estimation for the density determination, the contributions from the influence quantities are needed, specifically the weights of the part in water and air as well as the densities of the part in water and air. To determine these contributions, standard uncertainties are required.

3.2.1 Standard Uncertainty of Weights

Error sources that contribute to the uncertainty in the weight of the parts are a combination of systematic biases and random fluctuations. In hydrostatic weighing, the apparatus consists of a balance and suspension system. Significant systematic biases are the calibration, resolution and linearity [7], [8] of the apparatus. As for the random fluctuations, repeatability and reproducibility are contributors. With the error sources identified, the standard uncertainties are determined by adding the sources in quadrature, where the standard uncertainty is estimated using Eq. 8,

$$u(W) = \left[\left(\frac{x_{CAL}}{k}\right)^2 + \left(\frac{x_{RES}}{\sqrt{6}}\right)^2 + \left(\frac{x_{LIN}}{\sqrt{3}}\right)^2 + x_{STD}^2\right]^{1/2} \tag{8}$$

The distributions assumed are reasoned as follows: the calibration quantity x_{CAL} is taken from the calibration certificate where the divisor k is the coverage factor determined by the calibration lab (i.e. $k = 1$ for 68%, $k = 2$ for 95% and $k = 3$ for 99%). Finite resolution, x_{RES}, attributes to the rounding error in measurements and has a tendency to be at or near the center of a distribution of measurements, therefore a triangular distribution best describes these tendencies. As for linearity, x_{LIN}, it is assumed 100% contained between the certification limits and equally probable of being anywhere within those limits, thus a uniform distribution assumed. Finally, the uncertainty contribution for the repeatability or reproducibility, x_{STD}, is determined using a normal distribution to identify the variability via a sample standard deviation. A sole contribution which may have a negligible effect, only for the uncertainty contribution from the weight in water, is linearity if a part mass of $500\ g$ or less is measured.

3.2.2 Standard Uncertainty of Water Density

The mathematical model for the density of water is a function of the effects of dissolved air and pressure [3]. Dissolved air takes into account the temperature of the water, T_W, and the interval of deaeration (removal of air molecules), t, while the pressure accounts for the compressibility of the water, C, the barometric pressure, B, and the immersion depth, I. The measurement model is shown below in Eq. 9,

$$\rho_W = \left[1 - \left(\frac{(T_W - 3.9863)^2}{508929.2}\right)\left(\frac{T_W + 288.9414}{T_W + 68.12963}\right)\right][0.999973] \times \left[\frac{1}{1 - C\left(\frac{B}{760} + \frac{I}{1033} - 1\right)}\right]\left[1 - (2.11 - 0.053T_W)\left(1 - \frac{1}{1+t}\right)(10^{-6})\right] \tag{9}$$

The first term for Eq. 9 is the Tilton-Taylor formula for ρ_W as a function of water temperature in grams/millimeter. The second term reduces their values to grams/cubic centimeters. The third term is a correction for pressure and the fourth term is for dissolved air. In reality, the last two terms are negligible and can be ignored since this would change ρ_W, at most, 1.5 ppm [3]. Environmental influences will have the largest effects on the density determination of the part in water, specifically the water temperature and barometric pressure. Simplifications are made to only account for these parameters. The simplification is shown in Eq. 10.

$$\rho_W = \left[1 - \left(\frac{(T_W - 3.9863)^2}{508929.2}\right)\left(\frac{T_W + 288.9414}{T_W + 68.12963}\right)\right][0.999973] \times \left[\frac{1}{1 - C\left(\frac{B}{760} + \frac{I}{1033} - 1\right)}\right]\underbrace{\left[1 - (2.11 - 0.053T_W)\left(1 - \frac{1}{1+t}\right)(10^{-6})\right]}_{\approx 1} \tag{10}$$

$$\downarrow$$

$$= \left[1 - \left(\frac{(T_W - 3.9863)^2}{508929.2}\right)\left(\frac{T_W + 288.9414}{T_W + 68.12963}\right)\right]\left[\frac{(0.999973)}{1 - C\left(\frac{B}{760} + \frac{I}{1033} - 1\right)}\right]$$

Next, the third term deals with the effects from pressure. Since the barometric pressure is one of two terms considered, the influence from the compressibility of water ($C \approx 48\,\frac{ppm}{atm} = 0.063\,\frac{ppm}{mmHg}$, [9]) is minimal since the change in volume due to pressure is near constant. As for the immersion depth, it is assumed that the part is immersed at approximately at the center of gravity of the density bath tank (Figure 1), theoretically determined to be 6.25" (15.88 cm) [10].

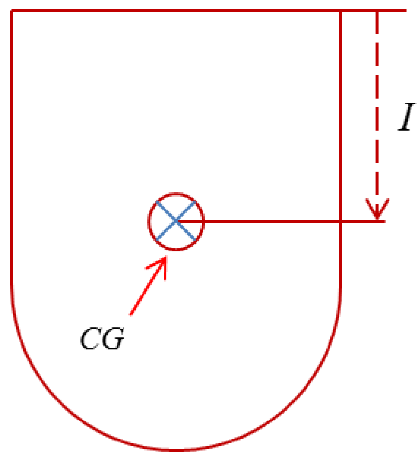

Figure 1: Immersion depth at center of gravity (CG), **[8]**.

Applying the values for the compressibility and depth of immersion to Eq. 10, the simplified model then becomes a function of the water temperature and barometric pressure as shown in Eq. 11 below,

$$\rho_W = \left[1 - \left(\frac{(T_W - 3.9863)^2}{508929.2}\right)\left(\frac{T_W + 288.9414}{T_W + 68.12963}\right)\right]\left[\frac{(0.999973)}{1 - 6.19 \times 10^{-8} B}\right] \quad (11)$$

where the uncertainty model is computed below in Eq. 12 using the LPU,

$$u(\rho_W) = \left[\left(\frac{\partial \rho_W}{\partial T_W}\right)^2 u^2(T_W) + \left(\frac{\partial \rho_W}{\partial B}\right)^2 u^2(B)\right]^{1/2} \quad (12)$$

and where the sensitivity coefficients for the water temperature and barometric pressure are computed below in Eq. 13,

$$\frac{\partial \rho_W}{\partial T_W} = \frac{63.4849T_W^3 + 15406.4T_W^2 + 1.2153 \times 10^6 T_W - 5.0932 \times 10^6}{(B - 1.6155 \times 10^7)(T_W + 68.1296)^2}$$

$$\frac{\partial \rho_W}{\partial B} = -\frac{1.2163 \times 10^{-13}[(T_W - 3.9863)^2(T_W + 288.941)]}{(1 - 6.19 \times 10^{-8}B)^2(T_W + 68.1296)} \quad (13).$$

The uncertainty contribution from the water temperature accounts for two sources: water temperature and the measurement sensor. For the water temperature, it is assumed to have a triangular distribution due to the part needing to reach thermal equilibrium with the water before measurements can be performed. As for the temperature sensor, the calibration uncertainty accounts for the contribution for a specific confidence interval (i.e., $k = 2$ at 95%), therefore,

$$u(T_W) = \left[\left(\frac{\Delta T_W}{\sqrt{6}}\right)^2 + \left(\frac{U_{95}(T_{W_{Sensor}})}{2}\right)^2\right]^{1/2} \quad (14).$$

For the barometric pressure uncertainty contribution, a similar approach is used where the range of potential values for the barometric pressure is assumed equally probable and 100% containment within the metrology lab's certified limits, thus a uniform distribution is assumed. Hence the uncertainty contribution is estimated as

$$u(B) = \left[\left(\frac{TOL_B}{\sqrt{3}}\right)^2 + \left(\frac{U_{95}(B_{Sensor})}{2}\right)^2\right]^{1/2} \quad (15).$$

3.2.3 Standard Uncertainty of Air Density

The density of the part in air is mathematically modeled as a function of environmental factors, namely ambient temperature, relative humidity and barometric pressure [3]. All laboratory measurements should be taken at the industry-standard of 20°C but ambient temperature fluctuations are periodic so the range can vary within the laboratory specification of $20.0℃ \pm \Delta T$. The model is shown in Eq. 16,

$$\rho_A = \frac{0.464554B - RH(0.00252T_A - 0.020582)}{T_A + 273.16} \quad (16)$$

where B is the barometric pressure, RH is the relative humidity and T_A is the temperature of air. It should be noted that this model represents measurements performed within a temperature range of 20°C to 30°C [11] and can be adjusted for the rare occasion of measurements performed outside this range [3], [9]. This adjustment for a wider temperature range makes the model go from linear to nonlinear; however, this will have a negligible effect somewhere in the range of $< 1\ \mu g/cm^3 = 1 \times 10^{-6}\ g/cm^3$. The uncertainty model is shown in Eq. 17,

$$u(\rho_A) = \left[\left(\frac{\partial \rho_A}{\partial B}\right)^2 u^2(B) + \left(\frac{\partial \rho_A}{\partial RH}\right)^2 u^2(RH) + \left(\frac{\partial \rho_A}{\partial T_A}\right)^2 u^2(T_A)\right]^{1/2} \tag{17}$$

where the sensitivity coefficients are shown below,

$$\frac{\partial \rho_A}{\partial B} = \frac{0.4646}{T_A + 273.16}$$

$$\frac{\partial \rho_A}{\partial RH} = \frac{0.0206 - 0.0025T_A}{T_A + 273.16} \tag{18}$$

$$\frac{\partial \rho_A}{\partial T_A} = -\frac{(0.4646B + 0.7089RH)}{(T_A + 273.16)^2}$$

The uncertainty contribution from barometric pressure is estimated using the same logic as it was for the part density in water, where it is assumed the pressure change is negligible between media. The relative humidity uncertainty contribution must account for the sensor uncertainty as well but for the actual barometric sensor, it is assumed equally probable and 100% containment within the metrology lab's limits, thus a uniform distribution is assumed. Therefore, the uncertainty can be estimated by

$$u(RH) = \left[\left(\frac{TOL_{RH}}{\sqrt{3}}\right)^2 + \left(\frac{U_{95}(RH_{Sensor})}{2}\right)^2\right]^{1/2} \tag{19}.$$

The uncertainty contribution from the air temperature accounts for two sources: air temperature and temperature sensor. For the air temperature, an uncertainty contribution is estimated using a U-distribution (arcsine) since HVAC systems recirculate room air in a cyclic manner which tends to keep the temperature closer to the maxima of the set points, hence

$$u(T_A) = \left[\left(\frac{\Delta T_A}{\sqrt{2}}\right)^2 + \left(\frac{U_{95}(T_{A_{Sensor}})}{2}\right)^2\right]^{1/2} \quad (20).$$

4.0 Example: Density of an Arbitrary Part

The following example is an application of determining the measurement uncertainty associated with the density determination of an arbitrary part. Suppose the part is repeatedly weighed 3 times, in water and in air, where the average values (and spreads) are $W_W = 1065.150 \pm 0.001\ g$ and $W_A = 1124.050 \pm 0.001\ g$. As for the systematic errors associated with the mass-balance, it is assumed that the mass balance used provides very accurate and precise results. For this mass balance, the following values are taken from the calibration certificate: $x_{cal} = 5 \times 10^{-5} g$ (at 95%, so $k = 2$), $x_{res} = 0.0001\ g$ and $x_{linear} = 0.0005\ g$. Therefore, the measurement uncertainties associated with the weights are estimated to be,

$$u(W_W) = \left[\left(\frac{5 \times 10^{-5}}{2}\right)^2 + \left(\frac{0.0001}{\sqrt{6}}\right)^2 + \left(\frac{0.0005}{\sqrt{3}}\right)^2 + (0.001)^2\right]^{1/2} = 0.001\ g$$

$$u(W_A) = \left[\left(\frac{5 \times 10^{-5}}{2}\right)^2 + \left(\frac{0.0001}{\sqrt{6}}\right)^2 + \left(\frac{0.0005}{\sqrt{3}}\right)^2 + (0.001)^2\right]^{1/2} = 0.001\ g \quad (21).$$

Next, the density of the part in both water and air are calculated. For these calculations, the environmental parameters used are $T_A = 20$°C, $T_W = 19.88$°C, $B = 586.74\ mmHg$, and $RH = 20\%$. Substituting in these values into Eq. 11, the density of the part in water is,

$$\rho_W = 0.9983\ \ g/cm^3 \quad (22).$$

The uncertainty is calculated using Eq. 12, where the sensitivity coefficients are,

$$\frac{\partial \rho_W}{\partial T_W} = -2.0503 \times 10^{-4}\ \ g/(cm^3 \cdot ℃)$$

$$\frac{\partial \rho_W}{\partial B} = -1.0782 \times 10^{-10}\ \ g/(cm^3 \cdot mmHg) \tag{23}$$

Assuming that $\Delta T_W = 0.5℃$, $U_{95}(T_{W_{Sensor}}) = 0.10℃$, $TOL_B = 72.6\, mmHg$ and $U_{95}(B_{Sensor}) = 0.15\, mmHg$, the standard uncertainty computed for the density of water is,

$$u(\rho_W) = \left[(2.0503 \times 10^{-4})^2 \left(\sqrt{\left(\frac{0.5}{\sqrt{6}}\right)^2 + \left(\frac{0.1}{2}\right)^2}\right)^2 + (1.0782 \times 10^{-10})^2 \left(\sqrt{\left(\frac{72.6}{\sqrt{3}}\right)^2 + \left(\frac{0.15}{2}\right)^2}\right)^2\right]^{1/2} = 4.3088 \times 10^{-5}\ \ g/cm^3 \tag{24}$$

For the density in air, the value is calculated using Eq. 16,

$$\rho_A = 0.9298\ \ mg/cm^3 = 9.297 \times 10^{-4}\ \ g/cm^3 \tag{25}$$

As for the uncertainty, the sensitivity coefficients are then computed,

$$\frac{\partial \rho_A}{\partial B} = 0.0016\ \ g/(cm^3 \cdot mmHg)$$

$$\frac{\partial \rho_A}{\partial RH} = -0.0001\ \ g/cm^3 \tag{26}$$

$$\frac{\partial \rho_A}{\partial T_A} = -0.0032\ \ g/(cm^3 \cdot ℃)$$

where the standard uncertainty is, assuming that $TOL_B = 72.6\ mmHg$, $U_{95}(B_{Sensor}) = 0.15\ mmHg$, $TOL_{RH} = 0.05$, $U_{95}(RH_{Sensor}) = 0.01$, $\Delta T_A = 1$°C and $U_{95}\left(T_{A_{Sensor}}\right) = 0.25$°C,

$$u(\rho_A) = \left[(0.0016)^2\left(\sqrt{\left(\frac{72.6}{\sqrt{3}}\right)^2 + \left(\frac{0.15}{2}\right)^2}\right)^2 + (0.0001)^2\left(\sqrt{\left(\frac{0.05}{\sqrt{3}}\right)^2 + \left(\frac{0.01}{2}\right)^2}\right)^2 + (0.0032)^2\left(\sqrt{\left(\frac{1}{\sqrt{6}}\right)^2 + \left(\frac{0.25}{2}\right)^2}\right)^2\right]^{1/2} = 6.6467 \times 10^{-5}\ g/cm^3 \tag{27}$$

With all the necessary values determined, the uncertainty of the arbitrary part density can be determined, where the sensitivity coefficients for Eq. 4,

$$\frac{\partial \rho_O}{\partial W_A} = -0.3062\ cm^{-3}$$
$$\frac{\partial \rho_O}{\partial \rho_W} = 19.0844\ (unitless)$$
$$\frac{\partial \rho_O}{\partial W_W} = 0.3231\ cm^{-3} \tag{28}$$
$$\frac{\partial \rho_O}{\partial \rho_A} = -18.0844\ (unitless)$$

Substituting in these values in to Eq. 6,

$$u_c(\rho_O) = [(-0.3062)^2(0.001)^2 + (19.0844)^2(4.3088 \times 10^{-5})^2 + \cdots + (0.3231)^2(0.001)^2 + (-18.0844)^2(6.6467 \times 10^{-5})^2]^{1/2}$$
$$\downarrow \tag{29}$$
$$u_c(\rho_O) = 0.0015\ g/cm^3$$

Assuming that the standard deviation of the repeated density measurements is $s(MP) = \pm 0.0020\ g/cm^3$, and taking the result from above, the total (expanded) uncertainty is

$$u_{Total}(\rho_O) = 2 \times [(0.0015)^2 + (0.0020)^2]^{1/2} = 0.005\ g/cm^3 \tag{30}$$

where evaluating the density of the part (Eq. 2) and stating the measurement uncertainty yields the final measurement result shown below,

$$\boldsymbol{\rho_O = (19.034 \pm 0.005)\ g/cm^3} \quad (31).$$

5.0 Conclusion

Updated uncertainty analysis for part density determination was presented, specifically using principles suggested by the GUM and sensitivity analysis to derive updated formulae. It should be noted that this does not always guarantee that small uncertainty values will be determined but does guarantee a more accurate statement as to how much uncertainty is associated with each measurement result. For the example provided, the original uncertainty value was determined to be $\pm 0.4455\ g/cm^3$ where the newly-determined uncertainty value using the revised formulae provided a fractional percentage of the original value. This is attributed to the larger uncertainty estimation from assuming that all the Type-B sources were normally-distributed at a confidence interval of 1-sigma and the sensitivities being derived with the use of total derivatives allowing for simultaneous variations.

6.0 References

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7.0 Appendices

7.1 Appendix A: Monte Carlo Simulation

An alternative approach to uncertainty estimations is via numerical simulations, specifically using Monte Carlo techniques. A general approach to simulating uncertainty estimations using Monte Carlo techniques is outlined in *Supplement 1* [12] where the influence quantities which make up the measurement model are assigned probability distributions and iterated for *N* trials. Figure 2 below shows the differences between the two uncertainty estimation methods suggested by the GUM.

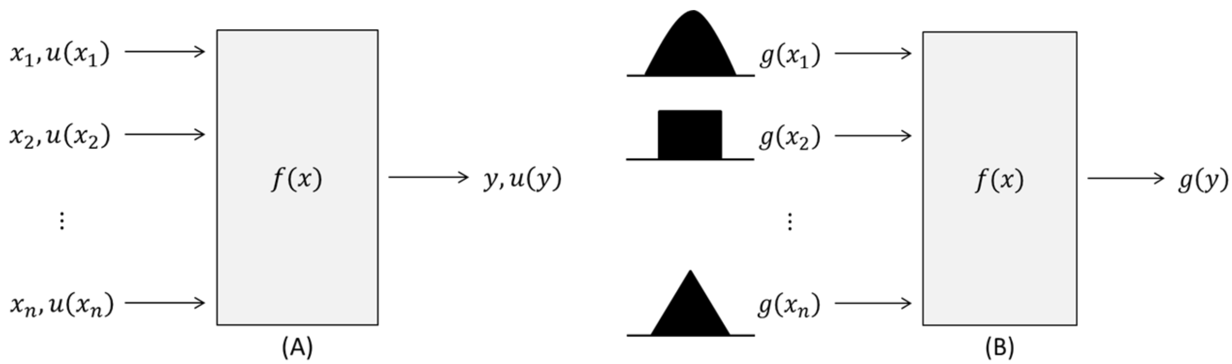

Figure 2: Illustrations of uncertainty methodologies: (A) propagation of uncertainties; and (B) propagation of distributions via Monte Carlo simulation.

Figure 2A is the propagation of uncertainties where the influence quantities (i.e. $x_1, x_2, \cdots, x_n$) and their respective uncertainties (i.e. $u(x_1), u(x_2), \cdots, u(x_n)$) are propagated through the model. With the restrictions set in place by the expectation values and variability, other potential information is lost. As for Figure 2B, no approximations are made and all the information from the input distributions are propagated throughout, however, the output is only as accurate as the input information.

Application of a Monte Carlo simulation can be performed with any software package which has a statistical toolbox. Routines in software packages like Excel, Matlab, Minitab, R and Python can be easily developed to perform these simulations but a simple, web-based alternative is the *NIST Uncertainty Machine* [13] (http://uncertainty.nist.gov/). This web-based software applies two different methods for uncertainty determination; Gauss's Linearization Formula (GUM) and Monte Carlo.

7.1.1 Example: Gauge Block Calibration

This example is taken from the GUM as an application of the NIST Uncertainty Machine. The length of a nominally 50 mm gauge block is determined by comparing it with a known reference standard of the same nominal length, also known as the Comparator Principle. The direct output of the comparison of the two gauge blocks is the difference d in their lengths given by

$$d = L(1 + \alpha\theta) - L_s(1 + \alpha_s\theta_s) \tag{A.1}$$

where L is the length at 20°C of the gauge block being calibrated, L_s is the length of the reference standard at 20°C from the calibration certificate; α and α_s are the coefficients of thermal expansion (CTE) for the gauge block being calibrated and the standard, respectively; θ and θ_s are the temperature deviations of the gauge block being calibrated and standard from 20°C, respectively.

The measurement model is that of the deviation of L from L_{nom} where after some algebraic manipulation, the model becomes,

$$\delta L = \frac{L_s[1 + \alpha_s(\theta_0 + \Delta - \delta\theta)] + D + d_1 + d_2}{1 + (\alpha_s + \delta\alpha)(\theta_0 + \Delta)} - L_{nom} \tag{A.2}$$

or approximately equal to,

$$\delta L = L_s + D + d_1 + d_2 - L_s[\delta\alpha(\theta_0 + \Delta) + \alpha_s\delta\theta] - L_{nom} \tag{A.3}$$

where D is the average of the five indications, d_1 and d_2 are the quantities describing, respectively, the random and systematic effects associated with using a comparator, $\delta\alpha$ is the difference in CTEs, θ_0 is a quantity representing the average temperature deviation of the gauge block from 20°C and Δ is a quantity describing the cyclic variation of the temperature variation from θ_0.

Table 1: Input quantities for gauge block model(s) and associated PDFs.

Quantity	***PDF***	***Parameters***				
		μ	σ	ν	a	b
L_s	$t_\nu(\mu, \sigma^2)$	$50.000623\ nm$	$25\ nm$	18		
D	$t_\nu(\mu, \sigma^2)$	$215\ nm$	$6\ nm$	24		
d_1	$t_\nu(\mu, \sigma^2)$	$0\ nm$	$4\ nm$	5		
d_2	$t_\nu(\mu, \sigma^2)$	$0\ nm$	$7\ nm$	8		
α_s	$R(a, b)$				$9.5 \times 10^{-6}\ ℃^{-1}$	$13.5 \times 10^{-6}\ ℃^{-1}$
θ_0	$N(\mu, \sigma^2)$	$-0.1℃$	$0.2℃$			
Δ	$U(a, b)$				$-0.5℃$	$0.5℃$
$\delta\alpha$	$R(a, b)$				$-1 \times 10^{-6}\ ℃^{-1}$	$1 \times 10^{-6}\ ℃^{-1}$
$\delta\theta$	$R(a, b)$				$-0.05℃$	$0.05℃$

With the measurement model complete, probability distributions can be assigned to each of the input quantities via the GUM, where Table 1 lists all the probability distribution functions (PDFs) and pertinent parameters. For the application shown here, the approximate model is used (Eq. A.3). Entering this information into the web-based interface and choosing the proper distributions is shown below in Figure 3,

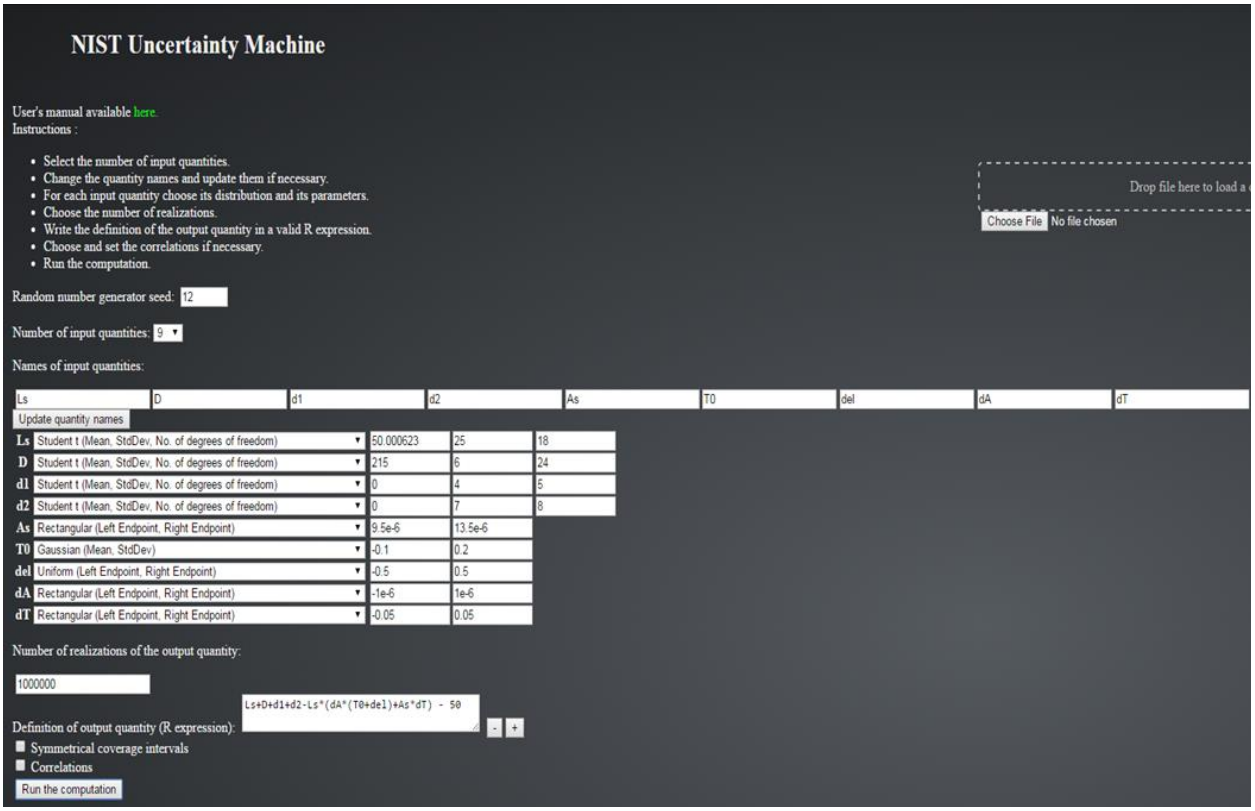

Figure 3: NIST Uncertainty Machine: Input parameters for gauge block calibration example.

where the results are shown below in Figure 4. Both the results for Gauss's linearization (GUM) and the Monte Carlo simulation are given. The value via Gauss's linearization yields $\delta L_{GUM} = (215 \pm 26.9)\ nm$ where the Monte Carlo simulation yields $\delta L_{MCS} = (215 \pm 27)\ nm$, basically identical results. Additional information, such as confidence intervals for the four standard percentages (i.e. 68%, 90%, 95% and 99%), are also provided with coverage factors based off the effective degrees of freedom. Furthermore, the plot shows the estimated probability density of the output quantity (solid blue line) and the probability density of a Gaussian distribution (dotted red line) with the same mean and standard deviation as the output quantity. In this case, the Gaussian approximation distribution is very accurate, as it closely fits to that of the distribution for the output quantity.

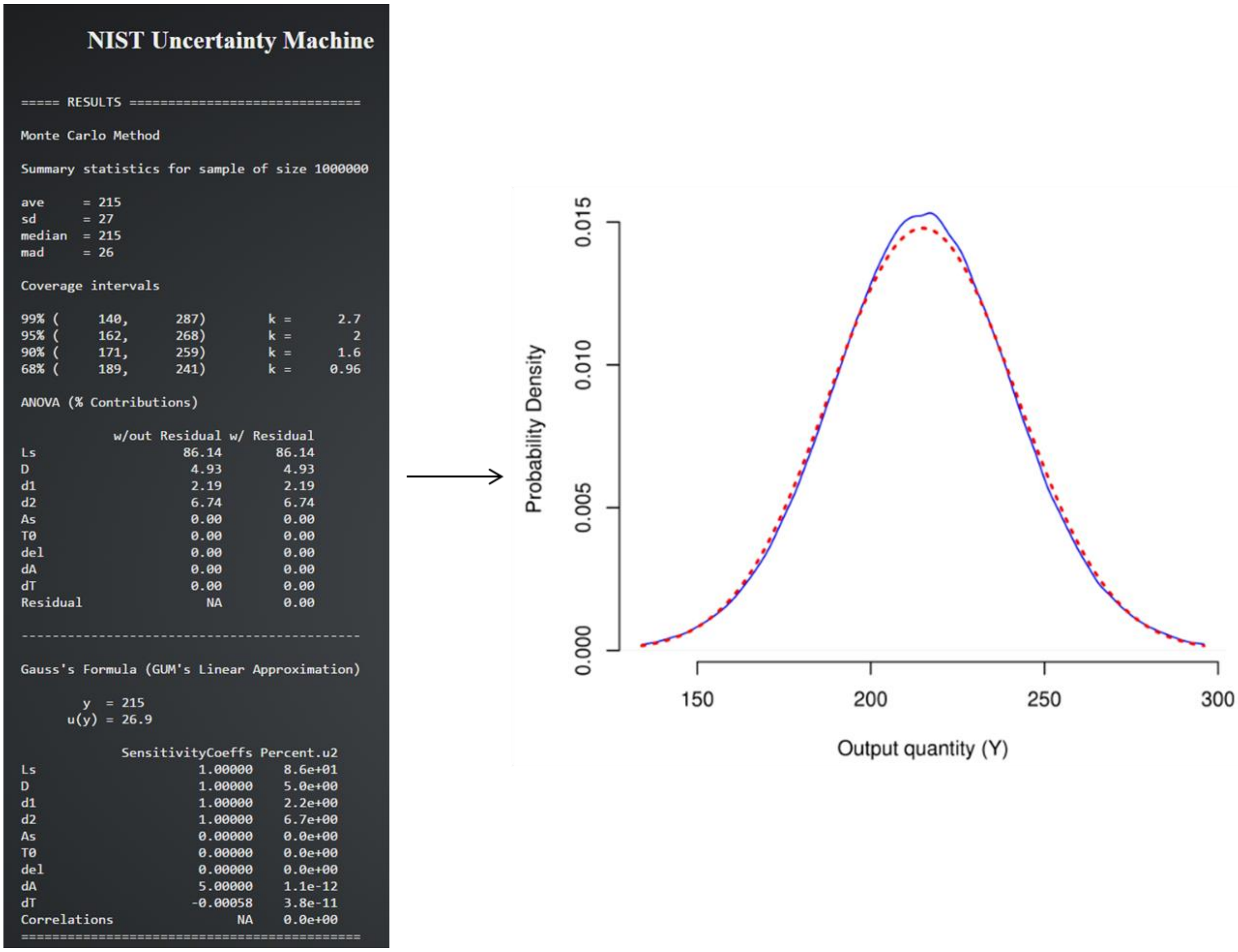

Figure 4: NIST Uncertainty Machine: Results for gauge block calibration.

The Monte Carlo approach works in a broader class of problems than that of the GUM, which in this sense is more general. However, it can be used to validate the results provided by the GUM since it is based on the same underlying principles. The main output of the Monte Carlo simulations is a coverage interval, not the standard uncertainty, hence the generality. Furthermore, the best-estimate (average) of the numerical approximation for the output distribution may not necessarily coincide with that provided by the GUM; this is the consequence of the different distributions used and the GUM aligning with the Student *t*-test (i.e. approximation of the *degrees of freedom* for the coverage factor).